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Power Transformations when the Choice of Power is Restricted to a Finite Set

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Abstract

We study the family of power transformations proposed by Box and Cox (1964) when the choice of the power parameter λ is restricted to a finite set Ω_R . The two cases in which obvious answers obtain are when the true parameter λ is an element of Ω_R and when λ is "far" from Ω_R . We study the case in which λ_0 is "close" to Ω_R , finding that the resulting methods can be very different from unrestricted maximum likelihood and that inference depends on the design, the values of the regression parameters, and the distance of λ to Ω_R .

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1. Introduction

Box and Cox (1964) suggested the power family of transformations, wherein for some unknown λ ,

(1.1)
$$y_i^{(\lambda)} = x_i \beta + \sigma c_i = \tau_i + \sigma c_i$$
, $i=1,...,N$.

Here the design vectors $x_i = (1 c_{i2} \dots c_{ip})$, $\beta = (\beta_0 \dots \beta_{p-1})$, the ϵ_i are independent and identically distributed with mean zero, variance one and distribution F, and

$$y^{(\lambda)} = (y^{(\lambda)} - 1)/\lambda$$
 $\lambda \neq 0$
= $\log y$ $\lambda = 0$.

They studied both maximum likelihood and Bayes inference when F is the normal distribution. There is now a substantial literature on the problem, an incomplete list of which includes Andrews (1971), Atkinson (1973), Hinkley (1975), Bickel and Doksum (1980, denoted B-D), Carroll (1980), and Carroll and Ruppert (1980, denoted C-R).

B-D developed an asymptotic theory for estimation. If the normal theory MLE is $\hat{\beta}$ when λ is known and $\beta^* = \hat{\beta}(\hat{\lambda})$ when λ is unknown and estimated by $\hat{\lambda}$, they compute the asymptotic distributions of $N^{1/2}(\hat{\beta} - \beta)/\sigma$ and $N^{1/2}(\beta^* - \beta)/\sigma$ as $N \rightarrow \infty$, $\sigma \rightarrow 0$. These distributions are different, with the latter having a covariance matrix at least as large and often very much larger than that of the former; the estimates $\hat{\lambda}$ and $\beta^{\#}$ are highly variable and highly correlated in general. This suggests that there is a large "cost" due to estimating the power parameter λ . Unfortunately, these results (and independent Monte-Carlo work by Carroll (1980)) suggest that unconditional inference concerning & can be very difficult for, balanced designs, inference without taking except in certain into account the variability of $\hat{\lambda}$ will be incorrect while β^* is itself too variable to be much help. A theory for conditional inference might prove useful.

It is relevant to note that when $\beta=0$ and $\sigma=1$ are known, the curvature (Efron (1975)) for λ at $\lambda=0$ is $\gamma_0^2=10.67$; Efron suggests that a value $\gamma_0^2\geq 1/8$ is "large"!

C-R study the prediction problem in the sense of estimating the conditional median of Y given a design point x_0 ; this is inference in the <u>original</u> scale of the data. Their results are much more encouraging; while there is a cost due to estimating λ , it is generally not severe. For example, if $\beta = (\beta_0 \ \beta_1 \ \dots \ \beta_{p-1})^{\frac{1}{2}}$, the cost averaged over the distribution of the design is $(1+p)^{-1}$ (asymptotically as $N \rightarrow \infty$ and $\sigma \rightarrow 0$).

We are concerned with the following point which has been raised concerning the applicability of the B-D and C-R theories. In practice, one may be uncomfortable using an estimate such as $\hat{\lambda}=.037$, then the much more common log scale $(\hat{\lambda}=0)$ is "just as good". Thus it is reasonable to restrict the estimate of λ to a finite set Ω_R and to study the consequences of such a decision. Asymptotically, as $N\to\infty$ but λ and Ω_R stay fixed, one has the trivial results that if $\lambda\in\Omega_R$ one is almost always in the right scale so there are no difficulties, while if $\lambda\notin\Omega_R$ bias dominates and no useful results are obtainable.

In Table I we present the results of a Monte-Carlo study for estimating the conditional median of Y given x_0 . The model is simple linear regression based on a uniform design with $\beta_0=5$, $\beta_1=2$ and

$$(1.2) N^{-1} \sum_{i=1}^{N} x_i' x_i = I_2.$$

The errors were normally distributed with mean 0 and variance σ^2 , and there were 500 replications of the experiment. The restricted power set was $\Omega_R = \{0, \pm 1/2, \pm 1\}$, and we made decisions in this set on the basis of the likelihood. For a given $\hat{\lambda}$, our estimator is

(1.3)
$$(1 + \hat{\lambda} \times_{o} \beta^{+})^{1/\hat{\lambda}} \qquad (\hat{\lambda} \neq 0)$$

$$\exp(\times_{o} \beta^{+}) \qquad (\hat{\lambda} = 0)$$

The numbers listed in the Table 1 are the "relative mean square errors (MSE)", i.e., the mean square error of (1.3) divided by the MSE when λ is known. We list results for the origen $x_0 = (1 \text{ o})$ and

when x_0 is a randomly chosen number of the design; the latter is in effect an average relative MSE over the distribution of the design.

In Table 1 we see that the restricted estimator (RE) dominates the MLE when $\lambda{=}0$ (hence $\lambda{\in}\Omega_{R}$), while the MLE dominates when $\lambda{\notin}\Omega_{R}$. In this latter case note that increasing N or decreasing σ results in improved performance of the MLE relative to the RE.

In Table 2 we repeat the above experiment with the changes β_0 =7, β_1 =4. The slightly worse behavior of the MLE relative to the λ -known case is expected from the C-R theory. Note here that the change in parameter values causes the RE to be much worse than the MLE if $\lambda \notin \Omega_R$. Also, the effect of changing N or σ is highlighted.

From the Monte-Carlo, we see that the performance of the RE relative to the MLE depends on λ , N, σ and β . One purpose of the rest of this paper is to propose and investigate a simple theory which gives a somewhat more systematic understanding of this performance. More generally, we also investigate the question of the feasibility of constructing procedures for which the choice of λ is restricted but which also give performance comparable to the MLE.

Table 1

The MSE behavior of the MLE and RE relative to the λ -known estimate of the conditional median of Y given $\mathbf{x_0}$. Here $\Omega_{\mathrm{R}} = \{0,\pm1/2,\pm1\}, \; \beta_0 = 5 \; \text{ and } \; \beta_1 = 2$.

 $\begin{array}{l}
\text{ORIGEN} \\
(\mathbf{x}_0 = (0.1))
\end{array}$

AVERAGE (x_o random member of design)

N	σ	λ	MLE	RE	Ratio (High/Low)	MLE	RE	RATIO
20	1	0	1.17	1.05	1.11	1.07	1.01	1.06
20	1/2		1.28	1.18	1.08	1.17	1.01	1.16
40	1		1.13	1.00	1.13	1.08	1.00	.1.08
40	1/2	0	1.22	1.00	1.22	1.16	1.00	1.16
20	1	1/8	1.13	1.26	1.12	1.07	1.15	1.07
20	1/2		1.25	1.43	1.14	1.13	1.24	1.10
40	1	}	1.12	1.29	1.15	1.03	1.10	1.07
40	1/2	1/3	1.25	1.53	1.22	1.05	1.24	1.18
							•	
20	1	1/4	1.12	1.17	1.04	1.06	1.10	1.04
20	1/2		1.24	1.34	1.08	1.12	1.24	1.11
40	1		1.10	1.29	1.17	1.04	1.10	1.06
40	1/2	1/4	1.23	1.52	1.24	1.06	1.14	1.08

Table 2

The MSE behavior of the MLE and RE relative to the λ -known estimate of the conditional median of Y given x_0 . Here $\Omega_R = \{0,\pm 1/2,\pm 1\}, \; \beta_0 = 7 \; \text{ and } \; \beta_1 = 4 \; .$

ORIGEN $(x_0 = (0 1))$

AVERAGE (x random member of design)

N	σ	λ	MLE	RE	Ratio (High/Low)	MLE	RE	RAT10
20	1	0	1.34	1,00	1.34	1.25	1.00	1.25
20	1/2		1.43	1.00	1.43	1.27	1.00	1.27
40	1		1.23	1.00	1.23	1.32	1.00	1.32
40	1/2	0	1.37	1.00	1.37	1.27	1.00	1.27
20	1	1/8	1.25	1.72	1.38	1.15	1.61	1.40
20	1/2		1.37	2.24	1.64	1.18	2.30	1.95
40	1		1.24	1.80	1.45	1.04	1.59	1.53
40	1/2	1/8	1.38	2.47	1.79	1.07	2.33	2.18
							`	
20	1	1/4	1.24	1.65	1.33	1.13	1.49	1.32
20	1/2		1.36	2.52	1.85	1.16	2.19	1.89
40	i		1.22	2.11	1.73	1.05	1.42	1.35
40	1/2	1/4	1.36	3.41	2.51	1.09	2.20	2.02

2. A large sample theory

Any reasonable theory must have λ "close" to Ω_R for large sample sizes. We choose to do this by letting the cardinality of Ω_R increase with increasing sample size N and by letting $\lambda = \lambda_N$ converge to a fixed element of Ω_R . For ease of calculation we focus on the important special case that the log scale is "almost" correct, i.e., Ω_R always contains zero and

$$\lambda = b\sigma/N^{1/2}$$

Of course, when b = 0 the data truely have a log-normal distribution.

Let $\hat{\lambda}_R$ and $\hat{\lambda}_M$ denote the restricted and ML estimates of λ , let $\hat{\beta}_R$ or β^* be the estimate of β having chosen the power $\hat{\lambda}_R$ or $\hat{\lambda}_M$, and let

$$f(\lambda, x_0 \beta) = (1 + \lambda x_0 \beta)^{1/\lambda} \qquad (\lambda \neq 0)$$

$$= \exp(x_0 \beta) \qquad (\lambda = 0),$$

which is the conditionional median of Y given x_0 , with estimate (1.2). We assume the errors are normally distributed. Letting $e = (1 \ 0 \ ... \ 0)$, we assume

$$\underline{x}_i e' = 1$$
 (there is an intercept)
 $N^{-1} \sum x_i' x_i = 1$:

Then, for any value of b, when λ is known the limit MSE is

(2.2)
$$MSE(\lambda \text{ known}) = \|x_0\|^2 \exp(2 x_0 \beta)$$
.

For fixed σ the computations are very difficult, so we will follow the lead of Bickel and Doksum and consider only the case that $\sigma = \Gamma \eta$, where $\Gamma = \Gamma(N) \to 0$ is a known sequence; it simplifies notation to make the convention $\eta = 1$.

We are now in a position to define the restricted estimate $\hat{\lambda}_R$ of λ , which we take by convention to satisfy $|\hat{\lambda}_R| \leq 1$. Let $\mathcal{D} = \{d_k\}$ be a finite or countably infinite subset of the extended real line with $|\hat{\lambda}_R| = 0$, $|\hat{\lambda}_R| = -|\hat{\lambda}_R|$, and $|\hat{\lambda}_R| = 0$. Define intervals midway between these points:

$$B_k = \left[(d_{k-1} + d_k)/2, (d_k + d_{k+1})/2 \right].$$

Our restricted estimate $\hat{\lambda}_R$ satisfies $|\hat{\lambda}_R| \leq 1$ and maximizes the likelihood over the admissible set with $|\hat{\lambda}_R| \leq 1$. Asymptotically, the procedure becomes

Choose $N^{1/2}\hat{\lambda}_R/\Gamma = d_k$ if $N^{1/2}\hat{\lambda}_M/\Gamma \in B_k$ and $|\hat{\lambda}_R| \le 1$. If not possible, choose $\hat{\lambda}_R = \pm 1$ on the basis of the likelihood.

The resulting estimate of β is $\hat{\beta}_R$ and the estimate of the conditional median of Y given x_o is $f(\hat{\lambda}_R, x_o \hat{\beta}_R)$.

The above procedure is asymptotically the same as a restricted maximum likelihood method and is quite intuitive as it choses the point in $\mathcal D$ closest to $N^{1/2}\hat{\lambda}_{M}/\Gamma$. Note also that as N increases, the number of possible choices for scale also increases, as desired. Make the definitions:

$$q_{N} = N^{-1} \sum_{i}^{N} \tau_{i}^{2} x_{i} \rightarrow q$$

$$a_{1} = [x_{o} q' - (x_{o}\beta)^{2}]/2$$

$$c_{N} = (-\tau_{i}^{2}/2 \dots -\tau_{N}^{2}/2)$$

$$x_{N}' = (x_{i}' \dots x_{N}')$$

$$e_{N} = (1/4) \{N^{-1} \sum_{i}^{N} \tau_{i}^{4} - \|q_{N}\|^{2}\} \rightarrow e_{o} > 0.$$

Theorem. Using the B-D asymptotics, the limit distribution of the restricted estimator of the conditional median

(2.1)
$$N^{1/2} \left[f(\hat{\lambda}_R, x_O \hat{\beta}_R) - f(\lambda = b\sigma/N^{1/2}, x_O \beta) \right]$$

is given by

(2.2)
$$\exp(x_0\beta) \left[\|x_0\| Z_1 + a_1 \sum_{k} (d_k - b) I(c_0^{-1/2} Z_2 + b \in B_k) \right]$$
,

where \mathbf{Z}_1 and \mathbf{Z}_2 are independent standard normal random variables. The proof is in the appendix.

The Theorem shows that the estimate of the conditional median of Y given \mathbf{x}_0 based on a restricted choice of λ is not necessarily asymptotically normally distributed.

Example $^{4+}1$. Suppose that for any sample size we restrict our choice of $\hat{\lambda}_R$ to a fixed set, say

$$\Omega_{\rm R} = \{0, \pm 1/2, \pm 1\}.$$

In this case we eventually have $\hat{\lambda}_{R} = 0$ so that $\mathcal{D} = \{0, \pm \infty\}$ and

(2.3) MSE (fixed finite set)

$$\Rightarrow \exp(2x_0\beta) \left[\|x_0\|^2 + b^2a_1^2 \right] .$$

In simple linear regression with a symmetric design and fourth moment μ_4 satisfying (1.2), we find that at the origen $\kappa_0 = (1 \text{ o})$, $a_1^2 = \beta_1^4/4$ and $e_0 = \beta_1^4 (\mu_4 - 1)/4$. In this case, while (2.3) does not serve as a very good method for predicting the individual values in Tables 1 and 2, it does, however, lead to the following qualitative conclusions, all of which are satisfied by the simulations:

- (i) Changing the value of N from 20 to 40 while fixing $\Omega_{\rm R}$ and λ basically increase b by a factor of $\sqrt{2}$. Hence, larger values of N will result in a worse performance for the RE when $\lambda \notin \Omega_{\rm R}$.
- (ii) Changing σ from 1 to 1/2 increases b by a factor of 2 and should result in worse performance for the RE.

- (iii) Changing P_1 from 2 to 4 increases the term B_1^4 by a factor of sixteen. Such a large change should cause much worse performance in Table 2.
- (iv) The increase in (iii) above should make the changes in the RE when one changes N or σ much more dramatic in Table 2 than in Table 1.

Example #2. The theory includes the MLE $\hat{\lambda}_{M}$ by choosing ν dense. In this case we get

(2.4a) MSE (MLE of λ)

$$+ \exp(2x_0 R) \left[\|x_0\|^2 + a_1^2/e_0 \right]$$
.

In the simple linear regression, at the origen this becomes

(2.4b)
$$\exp(2\beta_0)\left[1 + (\mu_4 - 1)^{-1}\right]$$
.

Note that (2.4h) is independent of the value of b.

Example #3. An interesting example in which the number of possible values of λ_R increases with N occurs when $\mathcal{D}=\{\text{all integers}\}$. It is not too unreasonable to suspect that this restricted estimate will be at least comparable to the MLE, perhaps somewhat better when b=0 and hence $\lambda\in\Omega_R$, but not too much worse when b = 1/2 and $\lambda\notin\Omega_R$. In this case

(2.5) MSE (restricted procedure)

$$+ \exp(2x_0^{\beta}) \left[\|x_0\|^2 + (a_1^2 e_0^{-1}) \sum_{k} (k-b)^2 e_0^{\beta} P\{e_0^{-1/2} Z + b \in B_k\} \right].$$

The only important difference between (2.4a) and (2.5) is the term

$$\sum_{\bf k} ({\bf k}^{-\bf b})^2 {\bf e}_{\bf o}^{\bf P} \{ {\bf e}_{\bf o}^{-1/2} z + {\bf b} \in B_{\bf k} \} \quad .$$

In Table 3 we compare the values of (2.4b) and (2.5) for the uniform simple linear regression design of the introduction with $\mu_4 = 1.79$; all comparisons are at the origen $x_0 = (1 \text{ o})$.

Table 3 Comparison of MSE for a simple linear regression design with moments $\mu_1 = \mu_3 = 0$, $\mu_2 = 1$, $\mu_4 = 1.79$, $\chi_0 = (1 o)$

b	<u>β</u> 1	MSE (MLE) MSE (λ known)	MSE (RE) MSE (λ known)	MSE (RE) MSE (MLE)
0	1.5	2.27	2.37	1.04
0	2.0	2.27	2.59	1.14
0	4.0	2.27	1.03	.45
1/2	1.5	2.27	2.37	1.04
1/2	2.0	2.27	2.61	1.15
1/2	4.0	2.27	129.42	57.01

The results are somewhat surprising. First note that the case b=0 corresponds to situations in which λ truely belongs to the set Ω_R . The restricted estimate does not always outperform the MLE, although it does for large β_1 . What is even more interesting is the case b=1/2, which is one of the simplest cases in which λ is not in the set Ω_R although it is quite close. Here we see that the restricted procedure can perform very badly indeed.

Tables 1-3 and the Theorem thus suggest that if the number of possible choices of scale is only on the order of $N^{1/2}$, the performance of the resulting estimates will differ from estimates based on the MLE of λ , in some cases being better but in others being very much worse. If one has no prior belief or evidence that only a finite number of values of λ are possible, but rather in estimating the conditional median of Y given x_0 one wants to make only "reasonable" choices of λ while retaining MLE-type behavior, the number of possible choices of λ will have to be

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Append i x

We will use contiguity techniques (Bajek and Sidak (1978)). Let L_1 be the log-likelihood when b=0 and let L_2 be the log-likelihood for fixed b ± 0. Somewhat detailed calculations show that as $N\to\infty$, $\sigma\to0$, under the distribution L_1 with $\lambda=0$,

(A.1)
$$- (L_2 - L_1) = (b^2/8N) \sum_{i=1}^{N} \tau_i^4 + (bN^{-1/2}) \sum_{i=1}^{N} \epsilon_i \tau_i^2/2 + o_p(1) .$$

This shows that the case $b \neq 0$ is contiguous to the case b = 0.

Proof of the Theorem: When $\lambda = b = 0$ it follows by a Taylor expansion in λ_R that as $N \to \infty$, $\sigma \to 0$

$$(\lambda.2) \qquad z_{N} = N^{1/2} \left[f(\hat{\lambda}_{R}, \hat{\beta}_{R}) - f(\lambda=0, \beta) \right] \exp(-x_{O}\beta)$$
$$= N^{-1/2} \sum_{i=1}^{N} x_{O} x_{i}^{i} \epsilon_{i} + a_{1} N^{1/2} \hat{\lambda}_{R} / \sigma + o_{p}(1) .$$

Also, B-D show that when $\lambda = 0$,

(A.3)
$$2e_0N^{1/2}\hat{\lambda}_M/\sigma = N^{-1/2}\sum_i (\tau_i^2 - x_iq^i)\epsilon_i + O_p(1).$$

It is easy to check that the r.h.s. of (A.3) is asymptotically independent of the first term on the r.h.s. of (A.2). We now use the definition of $\hat{\lambda}_R$ and the convention $\sigma = r(N)\eta = r(N)$ to obtain that when $\lambda = 0$, as $N \to \infty$ and $\sigma \to 0$,

(A.4)
$$S_N = N^{-1/2} \sum_{i=1}^{N} x_0 x_i^i \epsilon_i + a_1 \sum_{k} d_k I(N^{1/2} \hat{\lambda}_M / \sigma \in B_k) + o_p(1)$$
.

We are now in a position to use Theorem 7.2 of Roussas (1972, page 38). In his notation,

$$T_{N}' = N^{-1/2} \sum_{i=1}^{N} (x_{o} x_{i}^{!} \epsilon_{i} \quad q \quad x_{i}^{!} \epsilon_{i} \quad \tau_{i}^{2} \epsilon_{i})$$
(A.5)
$$\Gamma = E T_{N} T_{N}'$$

$$h' = (0 \quad 0 \quad -b/2)$$
.

One can show that the terms in (A.5) satisfy the conditions of Roussas' Theorem 7.2 so that when $\lambda = b \sigma N^{-1/2}$, as $N \to \infty$ and $\sigma \to 0$, T_N is asymptotically normally distributed with mean. The and covariance Γ . Because of (A.3), this means that $N^{1/2} \hat{\lambda}_M/\sigma$ and the first term on the r.h.s. of (A.2) are, when $\lambda = b \sigma N^{-1/2}$, jointly asymptotically normally distributed with means (b. $-bx_0q/2$), variances $(e_0^{-1}, \|x_0\|^2)$ and zero covariance. From this we obtain that (2.1) is asymptotically distributed with the same distribution as

$$\|\mathbf{x}_0\|_{\mathbf{Z}_1} - b\mathbf{a}_1 + \mathbf{a}_1 \sum_{k} \mathbf{d}_k \mathbf{1} (e_0^{-1/2} \mathbf{z}_2 + \mathbf{b} \in \mathbf{B}_k)$$
,

where \mathbf{Z}_1 and \mathbf{Z}_2 are as in the Theorem. This completes the proof.